Determinant Quantum Monte Carlo Study of the Orbitally Selective Mott Transition

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We study the conductivity, density of states, and magnetic correlations of a two dimensional, two band fermion Hubbard model using determinant Quantum Monte Carlo (DQMC) simulations. We show that an orbitally selective Mott transition (OSMT) occurs in which the more weakly interacting band can be metallic despite complete localization of the strongly interacting band. The DQMC method allows us to test the validity of the use of a momentum independent self-energy which has been a central approximation in previous OSMT studies. In addition, we show that long range antiferromagnetic order (LRAFO) is established in the insulating phase, similar to the single band, square lattice Hubbard Hamiltonian. Because the critical interaction strengths for the onset of insulating behavior are much less than the bandwidth of the itinerant orbital, we suggest that the development of LRAFO plays a key role in the transitions.

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Introduction: The problem of a strongly correlated band put in contact with a more weakly interacting one is of long-standing interest. In the case of the periodic Anderson model (PAM), for example, one orbital is completely free of interactions, while a second orbital is at the opposite extreme: it has no hopping from site-to-site (zero bandwidth) and instead has only an on-site hybridization V with the uncorrelated band. A competition between on-site singlet formation between electrons in the two different orbitals and RKKY mediated antiferromagnetic (AF) order occurs as a function of V, and a resonance in the density of states at the Fermi surface is present at the transition between these two regimes.

Recently there have been a number of studies,[1,2,3,5] mainly within dynamical mean field theory (DMFT)[6], of the general question whether two different bands can exist with one metallic and the other insulating, the so-called 'orbitally selective Mott transition' (OSMT). Alternate methods of treating the correlations of the impurity problem arising within DMFT, ranging from iterated perturbation theory[1] to Quantum Monte Carlo (QMC)[1,2] and exact diagonalization[3,4] yield different results. The form of the interband coupling and, specifically, whether the Hund's rule term is treated in an SU(2) symmetric way or only an Ising term is retained, was also thought to affect the results. By now it is established that, within DMFT and using the most accurate impurity solvers, an OSMT is possible. As might be expected, the narrow band becomes insulating first, as correlations increase, followed by the wide band. Attention has also focussed on the nature of the transitions which are, in general, believed to be first order.

The most well controlled theoretical work on the OSMT has been formulated within the framework of model Hamiltonians (multiband Hubbard models) whose simplicity allows for detailed and precise numerical studies. However, similar issues have also been addressed using a combination of electronic structure and many-body methods to describe real materials. The Cerium volume collapse transition[7] is one prominent example in which there is an interplay between the localized f and metallic d orbitals. As in the PAM, the orbitals see each other through hopping processes as well as interaction. Here, Kondo physics arising from singlet formation between electrons in the two bands plays a crucial role in the volume collapse transition[7,8]. Similar OSMT physics occurs in other materials, $Ca_{2-x}Sr_xRuO_4$ being especially well studied[9].

The range of different conclusions which arise depending on the treatment of the many body correlations within DMFT suggests that there is a crucial need to examine also the role of the local DMFT approximation itself. In this paper we use determinant Quantum Monte Carlo (DQMC) to study the OSMT. This method allows us to test rigorously the effect of ignoring momentum dependence in the self-energy within DMFT as well as to examine the real space AF correlations which could form along with the Mott insulating transition.

Model and Computational Method: We consider a Hamiltonian in which there is one correlated electron band and a second orbital which is fully localized and represented by a set of spin-$\frac{1}{2}$ degrees of freedom,

$$\begin{aligned} H &= -t \sum_{\langle ij\rangle\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) \\ &+ \sum_i \Big[J_z S^z_i (n_{i\uparrow} - n_{i\downarrow}) + J_\perp (S^+_i c^\dagger_{i\downarrow} c_{i\uparrow} + S^-_i c^\dagger_{i\uparrow} c_{i\downarrow}) \Big] \\ &+ U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) \end{aligned} \quad (1)$$

Here t allows the hopping of electrons of spin σ between adjacent sites $\langle ij\rangle$ of a square lattice, with $c^\dagger_{i\sigma}(c_{i\sigma}, n_{i\sigma})$ the associated creation (destruction, number) operators. U is the on-site repulsion. We chose $t = 1$ as our energy scale. A chemical potential μ controls the filling. We set $\mu = 0$ which, by particle-hole symmetry, pins the density at half-filling, $\rho = 1$. These fermions are coupled to a set

of local spin-$\frac{1}{2}$ degrees of freedom S_i at each lattice site. In this paper we will restrict the Hund's rule interaction to the J_z term, as has been done by Costi *et al* in a recent DMFT study[10].

In the Hamiltonian Eq. 1 the local spins represent a highly localized orbital; hence the question of the possibility of an OSMT devolves to whether a metal-insulator phase change can occur in the remaining itinerant fermion orbital as the energy scales J and U are tuned. Eq. 1 is closely related to the Kondo lattice model, except that an on-site U is present for the electronic degrees of freedom, which is usually set to zero in the Kondo case. Changing U allows, potentially, for tuning through an OSMT. A number of experimental systems can be approximately described by such a mixture of electrons and spins[12]. There are other materials whose qualitative physics has been suggested to be described by Eq. 1, including $Ca_{2-x}Sr_xRuO_4$ where a spin-$\frac{1}{2}$ Ru ion moment coexists[10,11,13] with a metallic state near $x = \frac{1}{2}$.

Our methodology is a version of the DQMC[14] algorithm often used to study Hubbard Hamiltonians, modified to include the effects of the fluctuating local spin degrees of freedom which represent the localized band. These local spins, together with the Hubbard-Stratonovich (HS) field which decouples the interaction, specify the up and down spin determinants whose product acts as the weight for the combined HS and local spin configuration. The HS field depends on both the spatial site and on the imaginary time coordinate τ which arises when the inverse temperature β is discretized. The local spin, on the other hand, while varying in space, is constant in τ. The HS variables are updated with the usual fast algorithm which uses the fermion Green's function to compute the change in the determinant[14]. The local spin is updated with a variant of the approach used for 'global moves' to ensure ergodicity in the HS distribution in determinant QMC[15], since those moves were also developed to handle changes which are non-local in τ.

The possibility of an OSMT in Eq. 1 with $J_\perp = 0$ has been explored in the DMFT study of Ref. [10]. The local moment $\langle S_z^2 \rangle$ was found to increase rapidly at a critical value of interaction strength which is a decreasing function of J/U. At the weakest $J/U < 0.05$, $\langle S_z^2 \rangle$ exhibits kinks indicative of what proves to be a first order OSMT. The evolution of the local moment is smoother for larger J/U, as the OSMT becomes second order. In Fig. 1 we show the behavior of $\langle S_z^2 \rangle$ in our DQMC calculations. Consistent with DMFT, there is an interaction strength, which decreases as J/U increases, for which the local moment changes rapidly. Significantly, in the neighborhood of this U value, the system must be cooled to a lower temperature in order to reach the ground state, indicative of the competition between states of nearly degenerate energy which occurs at a phase boundary.

Within mean field theories, the local moment can act as an order parameter, since when fluctuations are neglected the distinction between the energy scales and physics associated with local moment formation and long range magnetic correlations is blurred. However, as is well known, the local moment often loses its sharp structure when spatial fluctuations are included, as is the case with the DQMC simulations reported here. We therefore now turn to other measurements which can signal the OSMT more clearly. A key conclusion of our paper is that these quantities demonstrate that the orbitally selective transition found in DMFT survives.

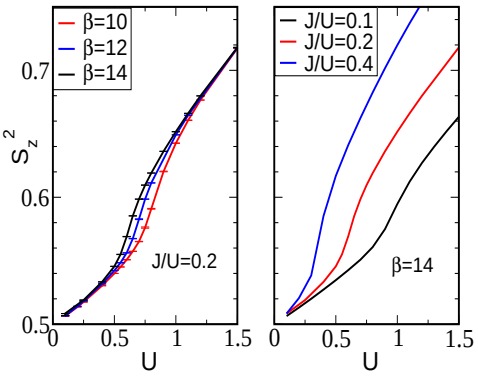

FIG. 1: (Color online) Left: The local moment $\langle S_z^2 \rangle$ of the correlated electron band is shown as a function of U for three different values of inverse temperature β for fixed $J/U = 0.2$. $\langle S_z^2 \rangle$ reaches its ground state value at $\beta < 10$ at weak and strong coupling and shows a roughly linear dependence on U. In the intermediate coupling regime, $\langle S_z^2 \rangle$ has an s-shaped form, and continues to evolve as T is lowered. Right: The transitional s-shaped structure in $\langle S_z^2 \rangle$ is seen to move to weaker coupling as J/U increases at fixed $\beta = 14$. The system is half-filled and size is 8x8.

Density of States: DQMC allows the direct measurement of the space and imaginary time Green's function and two particle correlation functions, Frequency dependent quantities can be obtained through a maximum entropy analytic continuation procedure[16] which inverts the integral relation between ω and τ.

Fig. 2(left) shows the density of states at the Fermi surface $A(0)$ for fixed $J/U = 0.2$. We see that as $T \to 0$, $A(0)$ is non-zero for $U/t < (U/t)_c \approx 0.5 \pm 0.1$. Above this critical value, the low temperature limit of $A(0)$ is zero. $(U/t)_c$ lies very close to onset point of U/t at which the local moment starts exhibiting pronounced temperature dependence, Fig. 1(left), as well as to the value $U/t \approx 0.6$ at which $\langle S_z^2 \rangle$ is changing most rapidly with interaction strength in Fig. 1(right).

Fig. 2(right) exhibits the energy dependence of $A(\omega)$. For U/t below the temperature crossing in Fig. 2(left), $A(\omega)$ has a maximum at $\omega = 0$, confirming this as a metallic state. By the time $U/t = 0.75$ this maximum has been replaced by a deep mimimum, almost to $A(0) = 0$. Indeed, if the temperature were lowered further a full gap would form, such as is seen for $U/t = 1.0$. Fig. 2(right) demonstrates that a OSMT occurs in the Hamiltonian

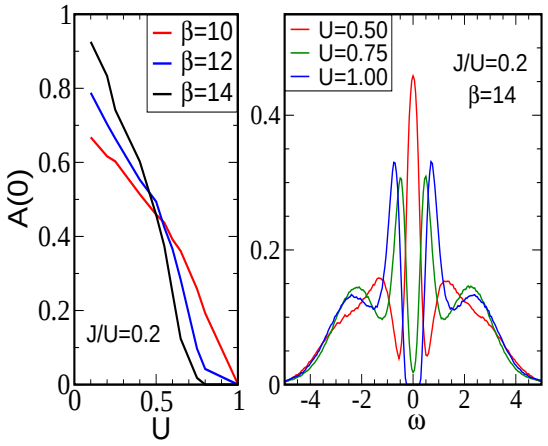

FIG. 2: (Color online) Left panel: The density of states at the Fermi surface $A(\omega = 0)$ of the weakly correlated orbital is shown as a function of the interaction U. Below $U/t = (U/t)_{\rm crit} \approx 0.5 \pm 0.1$, $A(0)$ rises as the temperature is lowered (β increases), indicative of metallic behavior of the weakly interacting band. At larger U, the trend is reversed and $A(0)$ is suppressed, signaling insulating behavior. Right panel: the full frequency dependence of the density of states $A(\omega)$ is shown for $J/U = 0.2$. $A(\omega)$ has a maximum at $\omega = 0$ for the weakest coupling. When $U/t = 0.75$, a deep suppression of $A(\omega)$ is seen at the Fermi surface, and the system is fully insulating by the time $U/t = 1.0$. In both panels, the lattice is half-filled and has 64 sites.

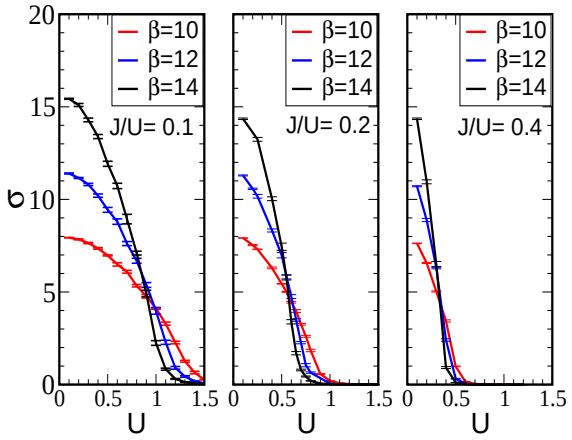

FIG. 3: (Color online) The dc conductivity $\sigma_{\rm dc}$ is shown as a function of interaction strength U/t for different values of the coupling between the itinerant and localized degrees of freedom. Left to right: $J/U = 0.1, 0.2, 0.4$. In all three cases, at weak coupling, $\sigma_{\rm dc}$ rises as the temperature T is lowered. As for the spectral weight at the Fermi surface (Fig. 2), this indicates the weakly correlated band is metallic. For U/t greater than a critical value, this trend with temperature reverses and the weakly correlated band undergoes an insulating transition. $(U/t)_c$ decreases as J/U increases. The lattice size is 8x8 and the filling $\rho = 1$.

Eq. 1. The size of the gap Δ in $A(\omega)$ is roughly U. However, one typically expects a gap set by U only deep in the Mott region where U exceeds the bandwidth $W = 8t$. As we shall discuss further below, we believe that here, instead, the gap Δ has a pronounced AF origin and is set by $Um_{\rm af}$ where $m_{\rm af}$ is the AF order parameter.

Conductivity: The dc conductivity $\sigma_{\rm dc}$ can be obtained from the large imaginary time dependence of the current-current correlation function[17]. We show the results in Fig. 3. As with the Fermi surface density of states, curves for different temperatures T cross when plotted as a function of U. The intersection demarks a transition from a metallic phase where $d\sigma_{\rm dc}/dT < 0$ to an insulating phase with $d\sigma_{\rm dc}/dT > 0$. The crossing point for $J/U = 0.2$ is consistent with the critical values obtained from $\langle S_z^2 \rangle$ (Fig. 1) and $A(0)$ (Fig. 2).

Magnetic Correlations: The presence of a gap in $A(\omega)$ even when U is an order of magnitude less than the bandwidth suggests that the insulating behavior does not arise purely from Mott physics- an energy lowering from avoiding double occupancy exceeding the cost in kinetic energy. We now explore the AF correlations which can give rise to a Slater gap in the spectrum.

Fig. 4 shows the AF structure factor $S_{zz}(\pi,\pi) = \frac{1}{N}\sum_{i,j}(-1)^{i+j}\langle S_i^z S_j^z \rangle$. When long range order is absent, the real space spin correlation $\langle S_i^z S_j^z \rangle$ decays exponentially. Only sites j within a correlation length ξ of site i contribute to the sum, and as a consequence, $S_{zz}(\pi,\pi)$, approaches a lattice size independent value at large N. $S_{zz}(\pi,\pi)\,/\,N$, shown in Fig. 4, therefore vanishes in the thermodynamic limit. On the other hand, in an ordered phase, the real space spin correlation $\langle S_i^z S_j^z \rangle$ is large for all pairs of sites i, j. The structure factor $S_{zz}(\pi,\pi)$, is

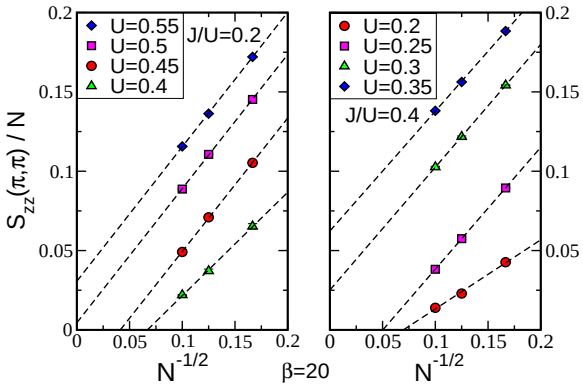

FIG. 4: (Color online) A finite size scaling plot of the antiferromagnetic structure factor shows that for $J/U = 0.2$ (left panel), long range order develops for U larger than $U_c \approx 0.5$. For $J/U = 0.4$ (right panel) there is a smaller $U_c \approx 0.3$.

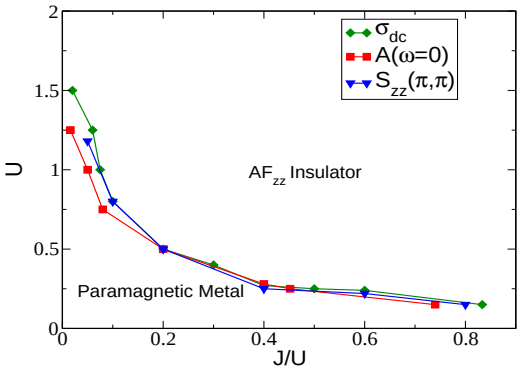

FIG. 5: (Color online) The phase diagram of the Hamiltonian Eq. 1, as determined by the various quantities measured in our simulation. At weak coupling (small J/U and U/t) there is a metallic phase.

proportional to N, and $S_{zz}(\pi,\pi)\,/\,N$, shown in Fig. 4, goes to a non-zero value. Huse[18] has used spin wave theory to make this argument more precise, and shown that $S_{zz}(\pi,\pi)\,/\,N = m_{\rm af}^2/3 + a/L$, where $L = N^{1/2}$ is the linear lattice size and $m_{\rm af}$ is the AF order parameter. In Fig. 4 we see that, at $J/U = 0.2$, for small U, less than $U_c \approx 0.5$, $S_{zz}(\pi,\pi)\,/\,N$ goes to zero for large N, while for U above this value there is long range order.

These results for long range magnetic order are consistent with the transition points observed in our early measurements. For example, in Fig. 3, at $J/U = 0.2$, when $U = 0.5$ (central panel), the system is metallic. When $J/U = 0.4$ and $U = 0.5$ (right panel), in contrast, the conductivity indicates insulating behavior. As expected, $\sigma_{\rm dc}$ goes to zero when there is long range AF order. Indeed, the size of the gap $Um_{\rm af}$ which would arise for electrons of one spin species moving through a staggered potential due to the other also matches well with the values seen in Fig. 2(right). It is important to note that the interaction term breaks spin rotation invariance, and hence we have this AF order only in the z direction. Finite size scaling of the xy AF structure factor indicates that the associated order parameter vanishes for all parameter regimes we have studied.

Conclusions: The complete ground state phase diagram in the $U - J/U$ plane is shown in Fig. 5. The different observables, $A(\omega = 0), \sigma_{\rm dc}$ and $S_{\rm zz}(\pi,\pi)$, all give (to within our error bars) a common phase boundary which separates a paramagnetic metallic phase from an insulating antiferromagnetic one. Generically, one expects the vertical ($J/U = 0$) axis, which corresponds to the usual Hubbard model, to be insulating above a critical value $U_{\rm c}$ (the Mott transition). Owing to the (logarithmically) divergent density of states, $U_{\rm c} = 0$ for a square lattice. However, this singularity is broken by a small nonzero J.

Magnetic correlations are known to have an important interplay with Mott physics both in the single band Hubbard Hamiltonian, and in the real materials for which it constitutes simple model. Similarly, in the single impurity and periodic Anderson Hamiltonians, local singlet formation and longer range AF order are central phenomena. In this paper, we have shown that in at least one model, the orbitally selective Mott transition is accompanied by the formation of a significant amount of intersite magnetic correlations, and that this inclusion of spatial fluctuations does not alter the qualitative physics- a set of itinerant fermions can coexist with a fully localized band. As with much earlier work[10], we have considered a simplified model which does not allow the full Hund's rule coupling between bands. Simulations with such a term in place involve the fermion sign problem and cannot at present be undertaken at low enough temperatures.

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